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Frequency evaluation for exponentially fitted Runge–Kutta methods

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Abstract

This paper can be seen as a further investigation of the frequency evaluation techniques which are very recently proposed by Ixaru et al. for exponentially fitted multistep algorithms for first-order ordinary differential equations (ODEs). The question answered was how the frequencies should be tuned in order to have a maximal benefit from exponentially fitted methods. In a previous paper, this frequency evaluation algorithm was successfully applied in a direct way to a second-order exponentially fitted Runge–Kutta (EFRK) method of collocation type but such a direct application is impossible for higher-order EFRK methods. To overcome this difficulty we develop an efficient extension of Ixaru's frequency evaluation algorithm for the exponentially fitted RadauIIA method of third order. It is an adaption of Ixaru's algorithm in the sense that instead being applied globally, it is applied stagewise. Numerical experiments illustrate the properties of the developed algorithm.

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1. Introduction

The idea of using a basis of functions other than polynomials has a long history, going back at least to the papers [5,8,12] for exponential-type solutions. Gautschi [11] was concerned with the case of periodic or oscillatory solutions where the frequency, or some suitable substitute, can be estimated in advance. All his derived methods integrate exactly appropriate trigonometric polynomials of given order, just

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as classical methods integrate exactly algebraic polynomials of given degree. Another good theoretical foundation for the exponential fitting technique was given in [21]. Since then a lot of exponentially fitted (for short: EF) linear multistep methods have been constructed and most of them were developed for second-order differential equations where the first derivative is absent, and applied to solve equations of Schrödinger type. Also for first-order equations special tuned algorithms have been constructed. The question is how the frequencies must be chosen in order to have a maximal benefit of EF methods. The answer is recently given in [15–17] for EF multistep methods. An algorithm for EF multistep methods was presented in order to tune the frequencies numerically to be as optimal as possible for first order differential equations or for systems of such equations. By this action one order of accuracy is gained with respect to the underlying classical method. An important conclusion after this series of papers is that the optimal frequencies does not reflect the very solution but the behaviour of some higher-order derivatives of it. Another crucial consequence for EF methods is that their applicability is much larger as thought before. This consequence is perhaps one of the most surprising facts in the theory of EF methods and it can provide the theory a new dynamic. Some well-known stiff problems like the Robertson and HIREs equations, which have no connection with oscillating problems, have been solved with frequency evaluation algorithms [17]. On the other hand, EF algorithms were originally introduced for the efficient numerical integration of problems with oscillating or periodic solutions.

The study of exponentially fitted Runge–Kutta (EFRK) methods is a relatively new development and rather limited. We refer to the papers [7,22–24,26] as the most essential ones appeared in this field. In [29], the frequency evaluation procedure of Ixaru et al. is applied to a second-order EFRK method of collocation type in a straightforward way. For higher-order EFRK methods it is not possible to apply this procedure in its present form. Our intention is to extend Ixaru's frequency evaluation algorithm for some specific EFRK methods. We will show that an efficient extension can be made when the internal stages and the final stage are tuned on two separate frequencies. The paper is organized as follows: in Section 2, we give a short introduction to EFRK methods, some basic concepts of frequency evaluation for EFRK methods and a motivation for the construction of EFRK methods depending on two frequencies. In Section 3, we construct the third-order EFRadauIIA method based on two frequencies. In Section 4, we will give an extension of Ixaru's frequency evaluation algorithm for the new method. The linear stability is discussed in Section 5. In Section 6, some numerical examples show the efficiency of the new frequency evaluation algorithm and finally in Section 7 some conclusions are drawn.

2. Basic elements of the approach

2.1. EFRK methods

In the last decade much research has been performed in the area of the numerical solution of initial value problems (IVP) related to systems of first-order ordinary differential equations (ODE), i.e.

$$y' = f(x, y), \quad y(x_0) = y_0. \quad (2.1)$$

A s -stage Runge–Kutta (RK) method for the solution of (2.1) is a one-step method of the form

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i f(x_n + c_i h, Y_i)$$

with

$$Y_i = y_n + h \sum_{j=1}^s a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \dots, s.$$

A RK method is completely determined by means of its Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \quad \text{or equivalent by the triplet } (c, A, b),$$

where $c, b \in \mathbb{R}^s$, $A \in \mathbb{R}^{s \times s}$ and s denotes the number of stages of the RK method. Second-order ODEs may be expressed as first-order systems, or polynomial collocation may be used directly on the second-order problem. In either case, the resulting methods are Runge–Kutta–Nyström (RKN) methods. Several authors have constructed exponential fitted Runge–Kutta–(Nyström) (EFRK(N)) methods for which they claim that they exactly integrate exponential or trigonometric functions. The method in [24] was a first example of an explicit EFRK method of algebraic order four. It is worth to notice that this first presented technique is different from the exponential fitting techniques discussed in other papers on EFRK methods [9,10,22,23,26–30]. The construction of these EFRK methods are based on the *linear stage representation for RK methods* in Albrecht's approach [1,2]: each of the s internal stages and the final stage of a RK method can be seen as a linear multistep method on a nonequidistant grid and one can associate the following linear functionals:

- for the internal stages

$$\mathcal{L}_i[y(x); h; \mathbf{a}] = y(x + c_i h) - y(x) - h \sum_{j=1}^s a_{ij} y'(x + c_j h) \quad i = 1, 2, \dots, s, \quad (2.2)$$

- for the final stage

$$\mathcal{L}[y(x); h; \mathbf{b}] = y(x + h) - y(x) - h \sum_{i=1}^s b_i y'(x + c_i h). \quad (2.3)$$

For a given $y(x)$ appropriate to the solution of (2.1) the functionals (2.2)–(2.3) will lead to systems of linear equations $\mathcal{L}_i[y(x); h; \mathbf{a}] = 0$, $\mathcal{L}[y(x); h; \mathbf{b}] = 0$ with unknown A - and b -values. Paternoster [23] has first used Albrecht's approach for the derivation of implicit EFRK(N) methods of collocation type of low algebraic order which integrate exactly trigonometric polynomials of a given degree. On the other hand, Coleman [7] introduced mixed collocation methods for $y'' = f(x, y)$; the collocation functions are linear combinations of trigonometric functions and powers. In [30], an algorithm for the derivation of EFRK methods was proposed in the frame of the general procedure in [14]. This general scheme allows modifying some standard algorithms for derivatives, quadrature and differential equations with the aim of making them tuned on oscillatory or exponential functions. For the use of Ixaru's general procedure [14] it is necessary to choose a reference set of functions of the form

$$\{1, x, \dots, x^K, \exp(\pm \mu x), \dots, x^P \exp(\pm \mu x) \mid \mu \in \mathbb{R} \text{ or } \mu \in i\mathbb{R}\}. \quad (2.4)$$

In the case of RK methods the reference set for each internal stage can be different from the set chosen for the final stage. Demanding that the functionals (2.2)–(2.3) will vanish for the chosen functions will

result in systems of linear equations with unknowns A - and b -values. This has the consequence that the A - and b -values are μ -dependent.

2.2. Frequency evaluation

2.2.1. Introduction

For a long time there was no definite answer on the question how the frequencies must be tuned in order to obtain a maximal gain from EF methods. Ixaru et al. [15–17] have presented a frequency evaluation algorithm for EF multistep methods that is able to tune the frequency μ in the way that the principal local truncation error (PLTE) is vanished. This action will raise the order by one unit. Analysing the behaviour of the error is therefore a necessary stage. We refer to these papers for technical details and for some practical points. For short, the procedure consists in the algorithms A0, A1 and A2 that integrate exactly all the linear combinations from the reference set of functions

- Algorithm A0: $\{1, x, \dots, x^K\}$ (the classical method),
- Algorithm A1: $\{1, x, \dots, x^{K-1}, \exp(\mu x) \mid \mu \in \mathbb{R}\}$,
- Algorithm A2: $\{1, x, \dots, x^{K-2}, \exp(\pm \mu x) \mid \mu \in \mathbb{R} \text{ or } \mu \in i\mathbb{R}\}$,

whereby K is determined by the considered method. An efficient criterium for a choice between A1 and A2 in each integration point was presented. We remark that Algorithm A1 is not covered by the general procedure from [14] which is concerned with functions of form (2.4). In [29], this frequency evaluation algorithm was directly applied to a second-order EFRK method of collocation type. Such methods are called *optimal EFRK methods*.

2.2.2. Partitioned EFRK methods

The case of systems of differential equations needs a specific attention. An increase of order can only be obtained if the frequency μ is tuned on each equation. It was explained in [16] that this procedure does not increase the computational effort significantly for EF multistep methods. This is not true for EFRK methods due to its nonlinearity. For example, when solve a system of two equations we have to perform the frequency evaluation procedure for each equation. The first (second) frequency μ_1 (μ_2) is calculated in the way that the first (second) component of the PLTE is zero, but in general the second (first) component is different from zero. The numerical solution of the j th component ($j = 1, 2$) in the next integration point is given by

$${}^j y_{n+1} = {}^j y_n + h \sum_{i=1}^s b_i (\mu_j h)^j k_i(\mu_j h).$$

This has the direct consequence that the ${}^j k_i$ -values have to be solved for each frequency μ_j and clearly the computational effort increase significantly. In order to overcome this difficulty we will use a *partitioned RK* (PRK) method [13]. A PRK method can be applied to a IVP of the form

$$\begin{aligned} y' &= f(x, y, z), & y(x_0) &= y_0, \\ z' &= g(x, y, z), & z(x_0) &= z_0, \end{aligned} \tag{2.5}$$

where y and z can be vectors of different dimensions. A RK method is partitioned if

$$\begin{aligned} y_{n+1} &= y_n + h \sum_{i=1}^s b_i k_i, \\ z_{n+1} &= z_n + h \sum_{i=1}^s \hat{b}_i \hat{k}_i, \\ k_i &= f \left(x_n + c_i h, y_n + h \sum_{j=1}^s a_{ij} k_j, z_n + h \sum_{j=1}^s \hat{a}_{ij} \hat{k}_j \right), \\ \hat{k}_i &= g \left(x_n + \hat{c}_i h, y_n + h \sum_{j=1}^s a_{ij} k_j, z_n + h \sum_{j=1}^s \hat{a}_{ij} \hat{k}_j \right). \end{aligned} \quad (2.6)$$

The idea of a PRK method is to treat the y -variables with the RK method (c, A, b) and the z -variables with a second RK method $(\hat{c}, \hat{A}, \hat{b})$. This idea can be extended to more than two methods. We use a separate frequency for each component such that the EFRK method will become a partitioned method. Clearly, the computational effort for the calculation of k_i and \hat{k}_i is exactly the same as for the corresponding classical RK method. This approach is first used and discussed in [29,30], but the frequency evaluation algorithm in relation with EFRK methods of order $p > 2$ in a partitioned approach is not investigated so far.

2.2.3. Frequency evaluation for EFRK methods of order $p > 2$

To start with a fresh look into the things we consider the second-order optimal EFRK method derived in [29]. When we apply the A1 and A2 versions to the scalar equation $y' = f(x, y)$ then the PLTE is given by

$$\text{PLTE(A1)} = \frac{h^3}{36}(y^{(3)} - \mu y^{(2)}), \quad \text{PLTE(A2)} = \frac{h^3}{36}(y^{(3)} - \mu^2 y').$$

Just as in [16–18] the optimal frequencies in x_n are given by $\mu(\text{A1}) = y^{(3)}(x_n)/y^{(2)}(x_n)$ and $\mu(\text{A2}) = \sqrt{y^{(3)}(x_n)/y'(x_n)}$. Here, we are concerned with the EFRadauIIA method (case 1: fixed knot-points) of order three derived in [30]. In fact, only Algorithm A2 for this method was presented. When we apply the EFRadauIIA method based on A1 to the above given scalar equation then the PLTE reads (see (4.1)–(4.2)):

$$\text{PLTE(EFRadauIIA, } s = 2, \text{ A1)} = -\frac{h^4}{216}[y^{(4)} - \mu^2 y^{(2)} - 4f_y(y^{(3)} - \mu y^{(2)})].$$

For the calculation of the optimal frequency μ in the A1-case we immediately observe an insuperable difficulty: the equation $\text{PLTE} = 0$ is a quadratic equation with unknown μ and therefore it is possible that one finds complex values for the optimal frequency. This has no sense because the chosen frequency must be real in the A1-case. This has clearly the consequence that the frequency evaluation procedure directly applied to EFRadauIIA methods is no option. Our intention in this paper is to develop an extension of the frequency evaluation technique to overcome the above-illustrated difficulty. The key of this extension consists in constructing EFRK methods that depend on two frequencies instead of one frequency. Suppose

that we tune each internal stage on the reference set of functions $\{x, \exp(\mu_I x) \mid \mu_I \in \mathbb{R}\}$ and that the final stage is tuned on the set of functions $\{\exp(\pm \mu_F x) \mid \mu_F \in \mathbb{R} \text{ or } \mu_F \in i\mathbb{R}\}$. Applying the obtainable EFRK method $(c, A(\mu_I), b(\mu_F))$ to the scalar equation as given above we will find for the PLTE (see (4.1)–(4.2)):

$$\text{PLTE} = -\frac{h^4}{216}[y^{(4)} - \mu_F^2 y^{(2)} - 4f_y(y^{(3)} - \mu_I y^{(2)})].$$

It consists of a sum of two contributions coming from the internal stages and the final stage. At each integration point x_n the PLTE will become zero for the choice $\mu_I = y^{(3)}(x_n)/y^{(2)}(x_n)$ and $\mu_F = \sqrt{y^{(4)}(x_n)/y^{(2)}(x_n)}$. This easy example provides the motivation for constructing some EFRK methods depending on two frequencies. The possibility of working with separate frequencies for the internal stages and the final stage is due to the fact that the stage-order of the two-stage RadauIIA method is one unit lower than the order of the method. In the case of a system of n ODEs $2n$ optimal frequencies (μ_I, μ_F) are involved and we can form n different RK-schemes $(c, A(\mu_I), b(\mu_F))$ ($i = 1, \dots, n$) that must be used in the partitioned approach for RK methods described in the previous subsection.

There are several reasons why some parts of the frequency evaluation algorithm cannot be directly applied to higher-order EFRK methods but a detailed description and investigation of most of these problems falls outside the scope of this paper.

Remark. The study of the PLTE for RK methods is much more complicated than for multistep methods. For higher-order EFRK methods the length of the expression for the PLTE is increasing rapidly. The question if there exists a general theory for constructing the PLTE for a given EFRK method is still open. As an illustration of this difficulty we consider the two-stage EFGauss method (case 1: fixed knot-points) given in [30] (p. 229). All the stages integrate exactly functions of the form (2.4) with $K = 0$ and $P = 0$. According to [14] one should expect that the PLTE is obtained by a modification of the PLTE of the classical Gauss method where $y^{(n)}$ is replaced by $y^{(n)} - \mu^2 y^{(n-2)}$ ($n = 3, 4, 5$). On the contrary, the expression of the PLTE contains the term μ^4 . This phenomenon can be explained by the general theory on *variable coefficient RK methods* of collocation type from [22]. An application of Lemma 1 from [22] will lead to: $b_1 + b_2 = 1 + \mathcal{O}(h^4)$.

3. Construction of EFRK methods depending on two frequencies

In general, EF methods depending on more than one frequency are rarely described. EF Multistep methods with several frequencies have been around in early papers from [3,4,25]. These multistep codes are capable of integrating exactly unperturbed harmonic oscillator equations. To give another example we can refer to [18] where different frequencies are automatically adjusted in terms of the equations to be solved. Very recently, Vigo-Aguiar et al. [31] have proposed optimal frequencies of some (coupled) oscillators with different frequencies based on a Poincaré–Lindstedt perturbation technique. This was accomplished by using an adapted Bettis method depending on two frequencies.

In so much all the previously constructed EFRK methods are depending on one frequency. Although, the new EFRK methods proposed in this paper are depending on two frequencies, they are not capable of integrating exactly two unperturbed oscillators for the simple reason that—beside the fact that Algorithm

A1 will be involved—the internal stages and the final stage are treated with two separate frequencies. Thus for the new RK approach there is no connection with the above-cited papers.

3.1. A-values depending on μ_I

For each internal stage we consider the following algorithms.

3.1.1. Algorithm ISA1

Each internal stage is tuned on the reference set of functions

$$\{x, \exp(\mu_I x) \mid \mu_I \in \mathbb{R}\}.$$

Demanding that the functional (2.2) for the i th internal stage ($i = 1, 2$) is vanishing for the chosen functions we obtain systems of linear equations ($v_I = \mu_I h$) the form:

$$a_{i1} + a_{i2} = c_i,$$

$$a_{i1} \exp(c_1 v_I) + a_{i2} \exp(c_2 v_I) = \frac{\exp(c_i v_I) - 1}{v_I}.$$

The following solution for the A-values is obtained for $c_1 = \frac{1}{3}$ and $c_2 = 1$:

$$\begin{aligned} a_{11} &= \frac{v_I \exp(v_I) - 3 \exp\left(\frac{v_I}{3}\right) + 3}{3v_I \left[\exp(v_I) - \exp\left(\frac{v_I}{3}\right) \right]}, & a_{12} &= \frac{3 \exp\left(\frac{v_I}{3}\right) - 3 - v_I \exp\left(\frac{v_I}{3}\right)}{3v_I \left[\exp(v_I) - \exp\left(\frac{v_I}{3}\right) \right]}, \\ a_{21} &= \frac{v_I \exp(v_I) - \exp(v_I) + 1}{v_I \left[\exp(v_I) - \exp\left(\frac{v_I}{3}\right) \right]}, & a_{22} &= \frac{\exp(v_I) - 1 - v_I \exp\left(\frac{v_I}{3}\right)}{v_I \left[\exp(v_I) - \exp\left(\frac{v_I}{3}\right) \right]}. \end{aligned} \quad (3.1)$$

For smaller values of $|v_I|$ the A-coefficients are subject of a heavy cancellation and we may use the next Taylor expansions:

$$\begin{aligned} a_{11} &= \frac{5}{12} - \frac{1}{27} v_I + \frac{1}{144} v_I^2 - \frac{19}{29160} v_I^3 + \frac{1}{38880} v_I^4 = \frac{1}{2204496} v_I^5 + \frac{11}{58786560} v_I^6 + \dots, \\ a_{12} &= -\frac{1}{12} + \frac{1}{27} v_I - \frac{1}{144} v_I^2 + \frac{19}{29160} v_I^3 - \frac{1}{38880} v_I^4 + \frac{1}{2204496} v_I^5 - \frac{11}{58786560} v_I^6 + \dots, \\ a_{21} &= \frac{3}{4} + \frac{1}{144} v_I^2 - \frac{1}{1080} v_I^3 + \frac{1}{38880} v_I^4 + \frac{1}{408240} v_I^5 + \frac{11}{58786560} v_I^6 + \dots, \\ a_{22} &= \frac{1}{4} - \frac{1}{144} v_I^2 + \frac{1}{1080} v_I^3 - \frac{1}{38880} v_I^4 - \frac{1}{408240} v_I^5 - \frac{11}{58786560} v_I^6 + \dots. \end{aligned} \quad (3.2)$$

3.1.2. Algorithm ISA2

Each internal stage is tuned on the reference set of functions:

$$\{\exp(\pm\mu_I x) \mid \mu_I \in \mathbb{R} \text{ or } \mu_I \in i\mathbb{R}\}.$$

Demanding that the functional (2.2) for the i th internal stage ($i=1, 2$) is vanishing for the chosen functions we obtain systems of linear equations ($v_I = \mu_I h$) of the form

$$\begin{aligned} a_{i1} \exp(c_1 v_I) + a_{i2} \exp(c_2 v_I) &= \frac{\exp(c_1 v_I) - 1}{v_I}, \\ a_{i1} \exp(-c_1 v_I) + a_{i2} \exp(-c_2 v_I) &= -\frac{\exp(-c_1 v_I) - 1}{v_I}. \end{aligned}$$

The following solution for the A -values is obtained for $c_1 = \frac{1}{3}$ and $c_2 = 1$ (see also [30]):

$$\begin{aligned} a_{11} &= \frac{(\alpha - 1)(\alpha^4 + \alpha^3 + \alpha^2 + \alpha + 1)}{v_I \alpha(\alpha + 1)(\alpha^2 + 1)}, & a_{12} &= -\frac{\alpha(\alpha - 1)}{v_I(\alpha + 1)(\alpha^2 + 1)}, \\ a_{21} &= \frac{(\alpha - 1)(\alpha^2 + \alpha + 1)^2}{v_I \alpha(\alpha + 1)(\alpha^2 + 1)}, & a_{22} &= \frac{(\alpha - 1)(\alpha^2 + \alpha + 1)}{v_I(\alpha + 1)(\alpha^2 + 1)}, \end{aligned} \quad (3.3)$$

where $\alpha = \exp(\frac{v_I}{3})$. For smaller values of $|v_I|$ it is preferable to use the following expansions:

$$\begin{aligned} a_{11} &= \frac{5}{12} + \frac{25}{1296} v_I^2 - \frac{5}{23\,328} v_I^4 + \frac{445}{35\,271\,936} v_I^6 - \frac{3179}{5\,714\,053\,632} v_I^8 + \dots, \\ a_{12} &= -\frac{1}{12} + \frac{7}{1296} v_I^2 - \frac{31}{116\,640} v_I^4 + \frac{2159}{176\,359\,680} v_I^6 - \frac{2263}{4\,081\,466\,880} v_I^8 + \dots, \\ a_{21} &= \frac{3}{4} + \frac{1}{144} v_I^2 + \frac{13}{38\,880} v_I^4 - \frac{709}{58\,786\,560} v_I^6 + \frac{587}{1\,058\,158\,080} v_I^8 + \dots, \\ a_{22} &= \frac{1}{4} - \frac{1}{144} v_I^2 + \frac{11}{38\,880} v_I^4 - \frac{731}{58\,786\,560} v_I^6 + \frac{589}{1\,058\,158\,080} v_I^8 + \dots. \end{aligned} \quad (3.4)$$

3.2. b -values depending on μ_F

For the final stage we consider the following algorithms.

3.2.1. Algorithm FSA1

Just like for ISA1 one should expect to obtain the next equations

$$\begin{aligned} b_1 + b_2 &= 1, \\ b_1 \exp(c_1 v_F) + b_2 \exp(c_2 v_F) &= \frac{\exp(v_F) - 1}{v_F}, \end{aligned}$$

but for practical reasons we replace the first equation by $b_1 c_1 + b_2 c_2 = \frac{1}{2}$ (the reason for this can be found in the structure of the error). This action is very unusual. However, we will illustrate in this paper that the obtained algorithm is useful. We have found for the b -values

$$b_1 = \frac{3(-v_F \exp(v_F) + 2 \exp(v_F) - 2)}{2v_F \left(3 \exp\left(\frac{v_F}{3}\right) - \exp(v_F)\right)}, \quad b_2 = \frac{3 \left(v_F \exp\left(\frac{v_F}{3}\right) - 2 \exp(v_F) + 2\right)}{2v_F \left(3 \exp\left(\frac{v_F}{3}\right) - \exp(v_F)\right)}. \quad (3.5)$$

For smaller values of $|v_F|$ the Taylor expansion must be used

$$\begin{aligned} b_1 &= \frac{3}{4} - \frac{1}{144} v_F^3 - \frac{1}{270} v_F^4 - \frac{29}{12\,960} v_F^5 - \frac{277}{204\,120} v_F^6 - \frac{3229}{3\,919\,104} v_F^7 - \frac{1837}{3\,674\,160} v_F^8 + \dots, \\ b_2 &= \frac{1}{4} + \frac{1}{432} v_F^3 + \frac{1}{810} v_F^4 + \frac{29}{38\,880} v_F^5 + \frac{277}{612\,360} v_F^6 + \frac{3229}{11\,757\,312} v_F^7 + \frac{1837}{11\,022\,480} v_F^8 + \dots. \end{aligned} \quad (3.6)$$

3.2.2. Algorithm FSA2

The final stage is tuned on the reference set of functions:

$$\{\exp(\pm \mu_F x) \mid \mu_F \in \mathbb{R} \text{ or } \mu_F \in i\mathbb{R}\}.$$

Demanding that the functional (2.3) will vanish for the chosen functions we obtain the linear system ($v_F = \mu_F h$):

$$\begin{aligned} b_1 \exp(c_1 v_F) + b_2 \exp(c_2 v_F) &= \frac{\exp(v_F) - 1}{v_F}, \\ b_1 \exp(-c_1 v_F) + b_2 \exp(-c_2 v_F) &= -\frac{\exp(-v_F) - 1}{v_F}. \end{aligned}$$

The solution is $b_1 = a_{21}$ and $b_2 = a_{22}$ whereby a_{21} and a_{22} are obtained from ISA2 and v_I is replaced by v_F .

3.3. Order conditions equations

Since there exist two possible algorithms for the internal stages and two possible algorithms for the final stage the EFRK method can be divided in four submethods. We denote a submethod based on ISA i and FSA j as (ISA i , FSA j) with $i, j = 1, 2$. It is interesting to check the algebraic order conditions well described in [13]. We check for the third order conditions for (ISA1, FSA2) to get

$$\begin{aligned} \sum_i b_i &= 1 + \frac{1}{1620} \mu_F^4 h^4 + \mathcal{O}(h^5), \\ \sum_i b_i c_i &= \frac{1}{2} - \frac{1}{216} \mu_F^2 h^2 + \frac{23}{58\,320} \mu_F^4 h^4 + \mathcal{O}(h^5), \end{aligned}$$

$$\sum_i b_i c_i^2 = \frac{1}{3} - \frac{1}{162} \mu_F^2 h^2 + \frac{7}{21\,870} \mu_F^4 h^4 + \mathcal{O}(h^5),$$

$$\sum_{i,j} b_i a_{ij} c_j = \frac{1}{6} + \frac{1}{54} \mu_I h - \left(\frac{\mu_I^2}{216} + \frac{\mu_F^2}{324} \right) h^2 + \left(\frac{7\mu_I^3}{14\,580} + \frac{\mu_F^2 \mu_I}{5832} \right) h^3 + \mathcal{O}(h^4).$$

EFRK methods containing ISA2 are violating the row-sum condition and in that case we have to put four additional conditions in order to confirm that the method is of third order. The following results are obtained for (ISA2, FSA1):

$$\sum_i b_i = 1 - \frac{1}{216} \mu_F^3 h^3 - \frac{1}{405} \mu_F^4 h^4 + \mathcal{O}(h^5),$$

$$\sum_i b_i c_i = \frac{1}{2},$$

$$\sum_{i,j} b_i a_{ij} = \frac{1}{2} + \frac{1}{54} \mu_I^2 h^2 - \frac{1}{4860} \mu_I^4 h^4 + \mathcal{O}(h^5),$$

$$\sum_i b_i c_i^2 = \frac{1}{3} + \frac{1}{648} \mu_F^3 h^3 + \frac{1}{1215} \mu_F^4 h^4 + \mathcal{O}(h^5),$$

$$\sum_{i,j,k} b_i a_{ij} a_{ik} = \frac{1}{3} + \frac{1}{81} \mu_I^2 h^2 + \frac{1}{648} \mu_F^3 h^3 + \left(\frac{23\mu_I^4}{43\,740} + \frac{\mu_F^4}{1215} \right) h^4 + \mathcal{O}(h^5),$$

$$\sum_{i,j} b_i a_{ij} c_i = \frac{1}{3} + \frac{1}{162} \mu_I^2 h^2 + \frac{1}{648} \mu_F^3 h^3 + \left(\frac{\mu_I^4}{29\,160} + \frac{\mu_F^4}{1215} \right) h^4 + \mathcal{O}(h^5),$$

$$\sum_{i,j,k} b_i a_{ij} a_{jk} = \frac{1}{6} + \frac{13}{648} \mu_I^2 h^2 + \frac{1}{1296} \mu_F^3 h^3 + \left(\frac{\mu_I^4}{174\,960} + \frac{\mu_F^4}{2430} \right) h^4 + \mathcal{O}(h^5),$$

$$\sum_{i,j} b_i a_{ij} c_j = \frac{1}{6} + \frac{5}{648} \mu_I^2 h^2 + \frac{1}{1296} \mu_F^3 h^3 + \left(-\frac{\mu_I^2}{6480} + \frac{\mu_F^2}{2430} \right) h^4 + \mathcal{O}(h^5).$$

It is clear that algorithms (ISA1, FSA2) and (ISA2, FSA1) are algebraically of third order, in the sense that

$$|y(x_n + h) - y_{n+1}| = \mathcal{O}(h^4).$$

Similar results are found for algorithms (ISA1, FSA1) and (ISA2, FSA2) but in the next section we will explain that both combinations will not occur in the new frequency evaluation algorithm.

4. Technical details for the extended frequency evaluation algorithm

4.1. Error analysis

The error of the EFRadauIIA method can be expressed as

$$\text{PLTE} = -\frac{h^4}{216}[B(\mu_F) + f_y A(\mu_I)], \quad (4.1)$$

whereby the expressions $A(\mu_I)$ and $B(\mu_F)$ depend on the choice of the algorithms given in Section 3, moreover the internal stages are responsible for $A(\mu_I)$ while $B(\mu_F)$ is determined by the final stage. This is reflected in the following expressions that we have found based on the order condition equations:

	<i>ISA1</i>	<i>ISA2</i>		<i>FSA1</i>	<i>FSA2</i>
$A(\mu_I)$	$y^{(3)} - \mu_I y^{(2)}$	$y^{(3)} - \mu_I^2 y^{(1)}$	$B(\mu_F)$	$y^{(4)} - \mu_F^3 y^{(1)}$	$y^{(4)} - \mu_F^2 y^{(2)}$

(4.2)

An increase of order is obtained when $\text{PLTE} = 0$ and therefore it is sufficient that $A(\mu_I) = B(\mu_F) = 0$. Both relations determine the optimal frequencies μ_I and μ_F for the considered algorithms.

4.2. Calculation of the derivatives

The evaluation of the optimal frequencies requires the knowledge of the total derivatives occurring in the expressions of the PLTE (4.1)–(4.2). This seems a very simple procedure: the first derivative is equal to the right-hand sides from (2.1) and the calculation of the higher derivatives is then just straightforward. This procedure works well for a lot of problems, but as explained in [16] it should be avoided on stiff problems. As also shown in [16], finite difference approximations of the derivatives are appropriate. Since the expressions of the PLTE given in (4.1) contain derivatives of order four we will approximate the derivatives in each integration point x_n by the following five-points finite difference formulae with at least an accuracy of $\mathcal{O}(h)$:

$$\begin{aligned} y^{(1)} &= \frac{-y_{n-3} + 6y_{n-2} - 18y_{n-1} + 10y_n + 3y_{n+1}^*}{12h} + \mathcal{O}(h^4), \\ y^{(2)} &= \frac{-y_{n-3} + 4y_{n-2} + 6y_{n-1} - 20y_n + 11y_{n+1}^*}{12h^2} + \mathcal{O}(h^3), \\ y^{(3)} &= \frac{y_{n-3} - 6y_{n-2} + 12y_{n-1} - 10y_n + 3y_{n+1}^*}{2h^3} + \mathcal{O}(h^2), \\ y^{(4)} &= \frac{y_{n-3} - 4y_{n-2} + 6y_{n-1} - 4y_n + y_{n+1}^*}{h^4} + \mathcal{O}(h). \end{aligned} \quad (4.3)$$

The data y_{n-3} , y_{n-2} , y_{n-1} and y_n for the input are the values of the numerical solution at x_{n-3} , x_{n-2} , x_{n-1} and x_n from the previous run and the estimation for the solution at x_{n+1} is denoted by y_{n+1}^* . This estimation is determined by the classical Milne–Simpson two-step formula [16]:

$$y_{n+1}^* = y_{n-1} + \frac{h}{3}(f(x_{n-1}, y_{n-1}) + f(x_n, y_n) + f(x_{n+1}, y_{n+1}^*)). \quad (4.4)$$

It is necessary that we make this approximation with a method that has a higher or the same order as the EF method. Therefore it is sufficient to choose the classical two-step Milne–Simpson method. It is clear that the above strategy for the calculation of the derivatives can only be started from the moment that in addition to the initial conditions in the point x_0 the solution is also known at the points x_1 and x_2 and x_3 .

4.3. Choosing between the algorithms

Algorithms ISA1 and FSA2 are not defined at x_n if $y^{(2)}(x_n) = 0$ while algorithms ISA2 and FSA1 are not defined if $y'(x_n) = 0$. In practice, we will observe very large values for the calculated frequencies and from then the frequency-determination technique will perform very badly. Just as in [16] a reasonable way of choosing between the algorithms in order to overcome high values for the frequencies consists in comparing $|y'(x_n)|$ and $|y^{(2)}(x_n)|$:

- If $|y'(x_n)| < |y^{(2)}(x_n)|$:
 - Algorithm (ISA1, FSA2) is selected.
 - The optimal frequencies are given by

$$\mu_I = \frac{y^{(3)}(x_n)}{y^{(2)}(x_n)}, \quad \mu_F = \sqrt{\frac{y^{(4)}(x_n)}{y^{(2)}(x_n)}}, \quad (4.5)$$

- If $|y'(x_n)| \geq |y^{(2)}(x_n)|$:
 - Algorithm (ISA2, FSA1) is selected.
 - The optimal frequencies are given by

$$\mu_I = \sqrt{\frac{y^{(3)}(x_n)}{y^{(1)}(x_n)}}, \quad \mu_F = \sqrt[3]{\frac{y^{(4)}(x_n)}{y^{(1)}(x_n)}}. \quad (4.6)$$

4.4. An overview of the extended procedure

- Starting the integration: the new frequency evaluation algorithm needs the value of the solution at four starting points x_0, x_1, x_2 and x_3 . We use a collocation method of order 5 [29, p. 353] for an accurate knowledge of the solution at x_1, x_2 and x_3 .
- The procedure for all other integration points: we start from x_n and we have to calculate the numerical solution at x_{n+1} .
 - Choosing between (ISA1, FSA2) and (ISA2, FSA1):
 - A good approximation for the solution at x_{n+1} is calculated by the classical Milne–Simpson two-step formula (4.4).

- The numerical solution at x_{n-3} , x_{n-2} , x_{n-1} and at x_n , calculated from a previous run and the value at x_{n+1} obtained by (4.4) are used for the approximation of the derivatives $y'(x_n)$, $y^{(2)}(x_n)$, $y^{(3)}(x_n)$ and $y^{(4)}(x_n)$ by means of five-points finite difference methods (4.3).
- Algorithms (IFA2, FSA1) or (FSA1, FSA2) are chosen in terms of the criterium given in Section 5.3.
- Evaluation of μ_I and μ_F : once the algorithm is chosen the optimal frequencies are determined by (4.5) or (4.6).
- Calculation of the μ_I -dependent A -values and the μ_F -dependent b -values given in Sections 4.1 and 4.2. For smaller values of $|v| = |\mu h| < v_0$ it is preferable to use the Taylor expansions of the A - or b -values whereby

	$ISA1$	$ISA2$	$FSA1$	$FSA2$
v_0	0.08	0.08	0.02	0.08

(4.7)

For systems of ODEs these stages are performed on each component.

- Calculation of the solution at x_{n+1} . For systems we use the partitioned approach for EFRK methods described in Sections 2.2.2 and 2.2.3. The EFRK method is fully implicit and a Newton–Raphson iteration is used.

5. Stability analysis

Linear stability analysis of numerical methods for first-order ODEs (2.1) is based on the test equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C}, \quad \operatorname{Re}(\lambda) < 0. \quad (5.1)$$

When a one-step method is applied to (5.1) it gives the difference equation

$$y_{n+1} = R(\hat{h})y_n \quad (5.2)$$

for the set of the numerical approximations y_n for the solution at $x_n = x_0 + nh$, whereby $\hat{h} = h\lambda$. We call $R(\hat{h})$ the *stability function*. If $n \rightarrow \infty$ then the numerical solution y_n will tend to zero iff

$$|R(\hat{h})| < 1. \quad (5.3)$$

The method is *absolute stable* for those values of $\hat{h} \in \mathbb{C}$ wherefore condition (5.3) holds. The region \mathcal{R}_A of the complex \hat{h} -plane wherefore (5.3) holds, is called the *region of absolute stability* of the method. The next definitions are taken from [19] and they are very important in relation with the numerical integration of stiff problems.

Definition 1. A one-step method wherefore the region of absolute stability contains \mathbb{C}^- is called A-stable.

However, A-stable methods can produce slowly damped oscillating errors. In order to overcome this difficulty one has introduced the concept of L -stability.

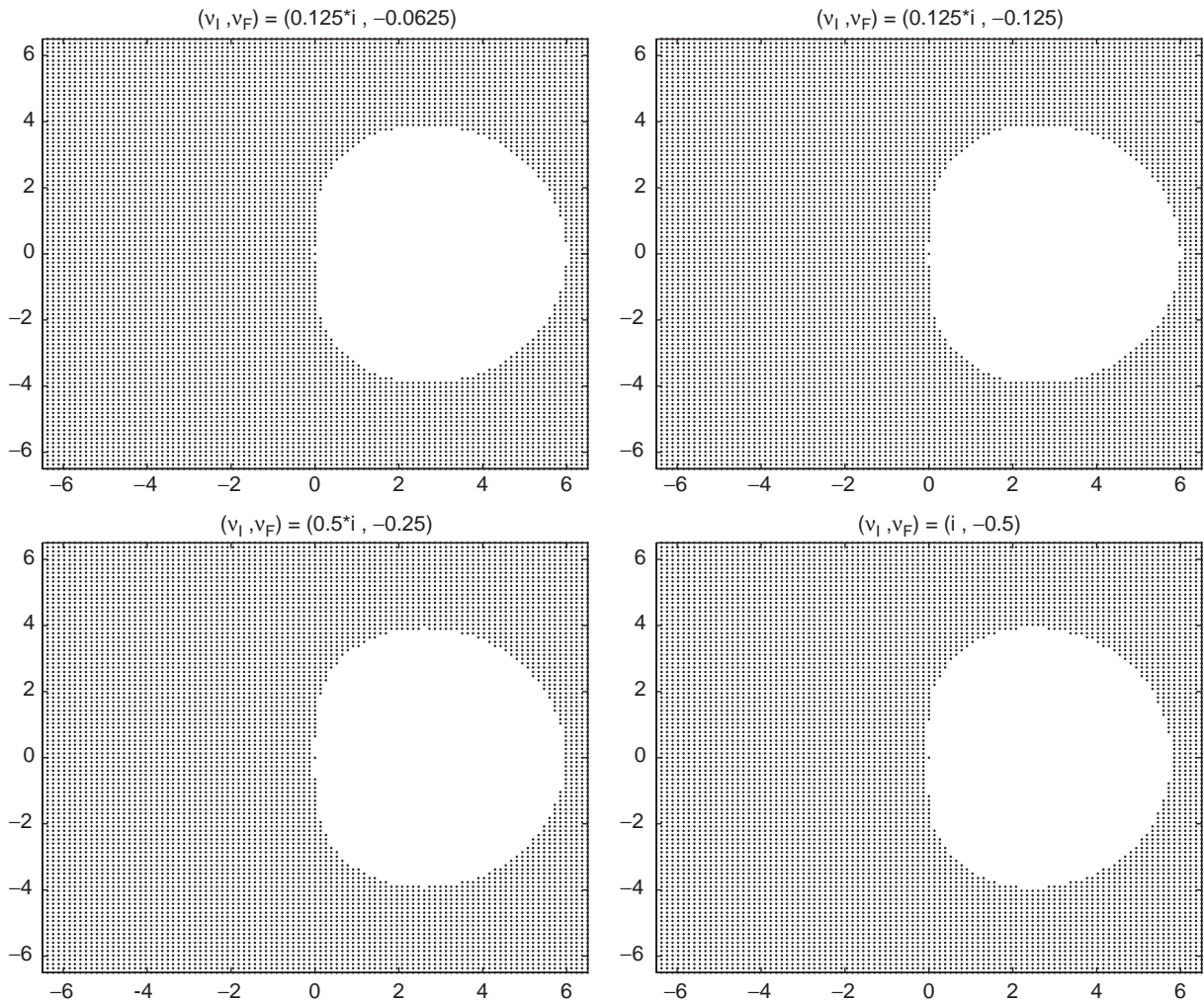


Fig. 1. Region of absolute stability for algorithm (ISA2, FSA1) at four values for the couple (v_I, v_F) .

Definition 2. A one-step method is called L-stable when the method is A-stable and moreover the next condition also holds:

$$\lim_{\hat{h} \rightarrow \infty} R(\hat{h}) = 0.$$

It seems that A- and L-stability are heavy conditions for RK methods. The following definition will relax the conditions for an A-stable RK method.

Definition 3. A one-step method is called $A(\alpha)$ -stable, $\alpha \in [0, \frac{\pi}{2}]$, if

$$\{\hat{h} \mid -\alpha < \pi - \arg \hat{h} < \alpha\} \subseteq \mathcal{R}_A.$$

Table 1

Errors $\Delta y_i(x) = |y_i(x) - y_i^{\text{comput}}(x)|$ at $x = 10$ for the two components ($i = 1, 2$) of Eq. (6.3), from the classical two-stage RadauIIA method and from the two-stage optimal EFRadauIIA method

h	$\beta = -3$		$\beta = -1000$	
	Δy_1	Δy_2	Δy_1	Δy_2
Classical RadauIIA method				
0.1	1.7E–5	4.5E–6	1.3E–5	1.8E–5
0.05	2.2E–6	5.7E–7	1.6E–6	1.3E–6
0.025	2.7E–7	7.3E–8	2.1E–7	1.4E–7
Optimal EFRadauIIA method				
0.1	2.7E–7	7.5E–7	3.0E–7	2.2E–7
0.05	1.4E–8	4.8E–8	1.8E–8	8.6E–9
0.025	7.7E–10	3.0E–9	1.1E–9	5.4E–11

Linear stability analysis is much more complicated for EFRK(N) methods than for the corresponding classical RK(N) methods, in which μ and h occur only in the combination $v = \mu h$. For EFRK(N) methods there are three parameters to consider, since the steplength h occurs both in $\hat{h} = \lambda h$, and $v = \mu h$. A first fruitful approach for the stability analysis (related to periodicity) of EFRKN methods of collocation type is given in [7]. Some stability properties can be proved for the EFRK collocation methods from [30]: an extensive study (which is not presented in this paper) learns that the EFLobattoIIIA method and EFGauss methods are A-stable $\forall v \in \mathbb{R}$. Thus these EFRK methods have the same stability properties as their underlying classical RK method. The EFRadauIIA method (case 1: fixed knot-points) is L-stable $\forall v \in \mathbb{R}$. In the case of pure imaginary frequencies (the trigonometric case) there is an alteration of the stability properties detected. Linear stability of EFRK methods is not described yet and we hope to report a stability analysis of previously derived (explicit and implicit) EFRK methods in a future paper. The situation becomes even more complex when we take into account that the EFRadauIIA method derived in this paper is depending on two different frequencies. The stability function is depending on \hat{h} , v_I and v_F and it is denoted as $R(v_I, v_F, \hat{h})$. Given the parameters (v_I, v_F) then $\hat{h} \in \mathbb{C}$ belong to the stability region if $|R(v_I, v_F, \hat{h})| < 1$. A systematic theoretical investigation of the stability properties for every couple of parameters would be near impossible. The only way to follow consists in drawing the regions of absolute stability at many values for the couple (v_I, v_F) and this may take a lot of experimentation. First, we notice that larger values $|v_I| > 1$ or $|v_F| > 1$ are rarely detected during our exploration of frequency evaluation algorithms applied to several (stiff) test problems. Now, we consider the submethod (ISA2, FSA1). We have experimentally derived that this method is L-stable for $-1 \leq v_I, v_F \leq 1$. The trigonometric case ($v_I \in i\mathbb{R}$) needs a specific treatment. In Fig. 1 we draw some regions of absolute stability for algorithm (ISA2, FSA1) at four values for the couple (v_I, v_F) ($v_I \in i\mathbb{R}$). We observe that a very small region in the neighbourhood on the imaginary axis does not belong to the region of stability. This means that the method in the trigonometric case (with $|v_I|, |v_F| \leq 1$) is A(α)-stable where α is depending on (v_I, v_F) . Similar results are found for the submethod (ISA1, FSA2). From all these considerations it is clear that it is safe to claim that we will not experience stability problems with the developed algorithm.

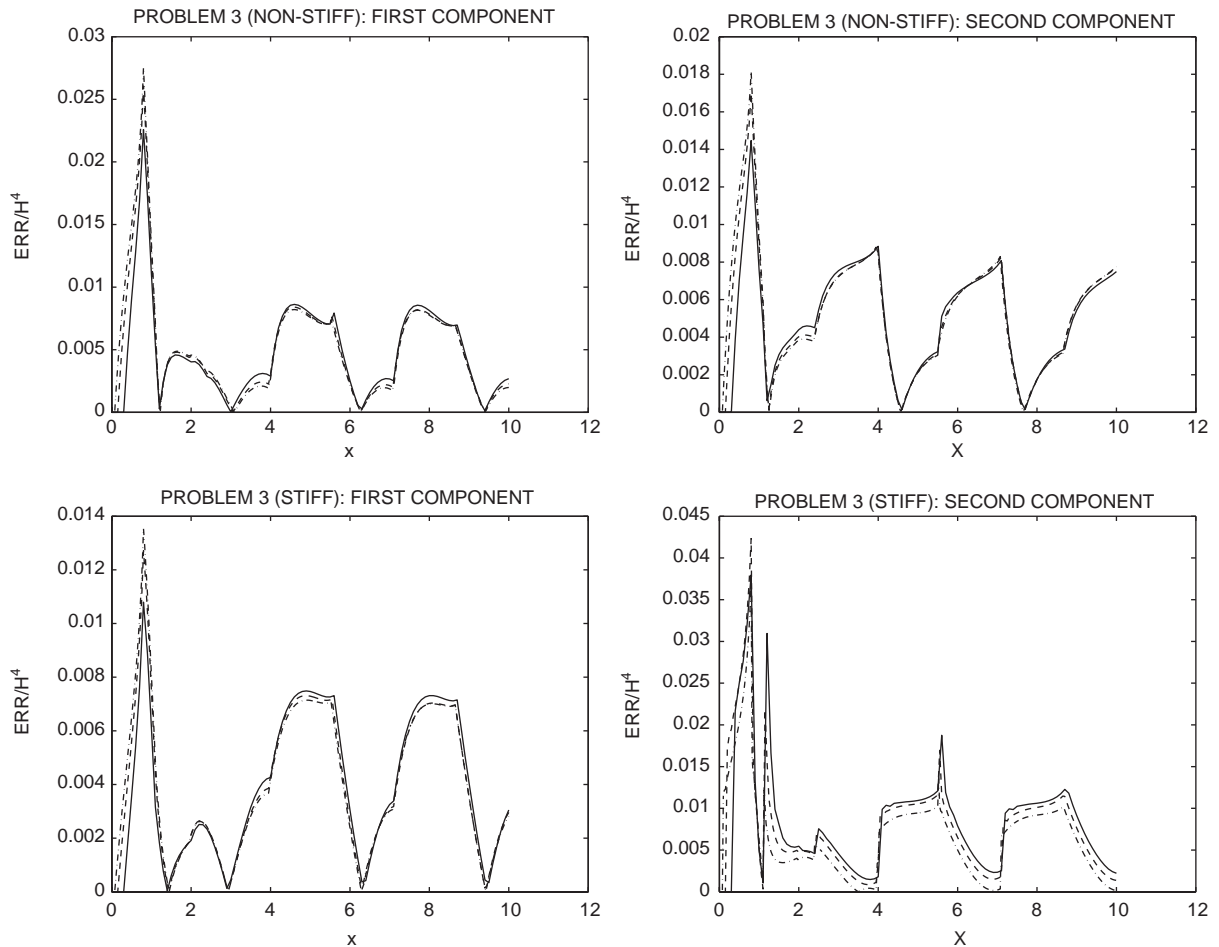


Fig. 2. Scaled errors $(y(jh) - y_j)/h^4$, $j = 1, 2, 3, \dots$ for the two-stage optimal EFRadauIIA method at three steplengths: $h = 0.1$ (solid line), $h = 0.05$ ('- -') and $h = 0.025$ ('.-') for the first and second component of Eq. (6.3) in the cases $\beta = -3$ (nonstiff) and $\beta = -1000$ (stiff). The initial conditions are given by (6.5).

6. Numerical illustrations

6.1. The test problems

Problem 1. We consider the following nonlinear first-order ODE studied by Chawla et al. [6]:

$$y' = \frac{y}{x} \ln(y), \quad y(0.5) = \exp(-1). \quad (6.1)$$

The domain of numerical integration is $[0.5, 3]$.

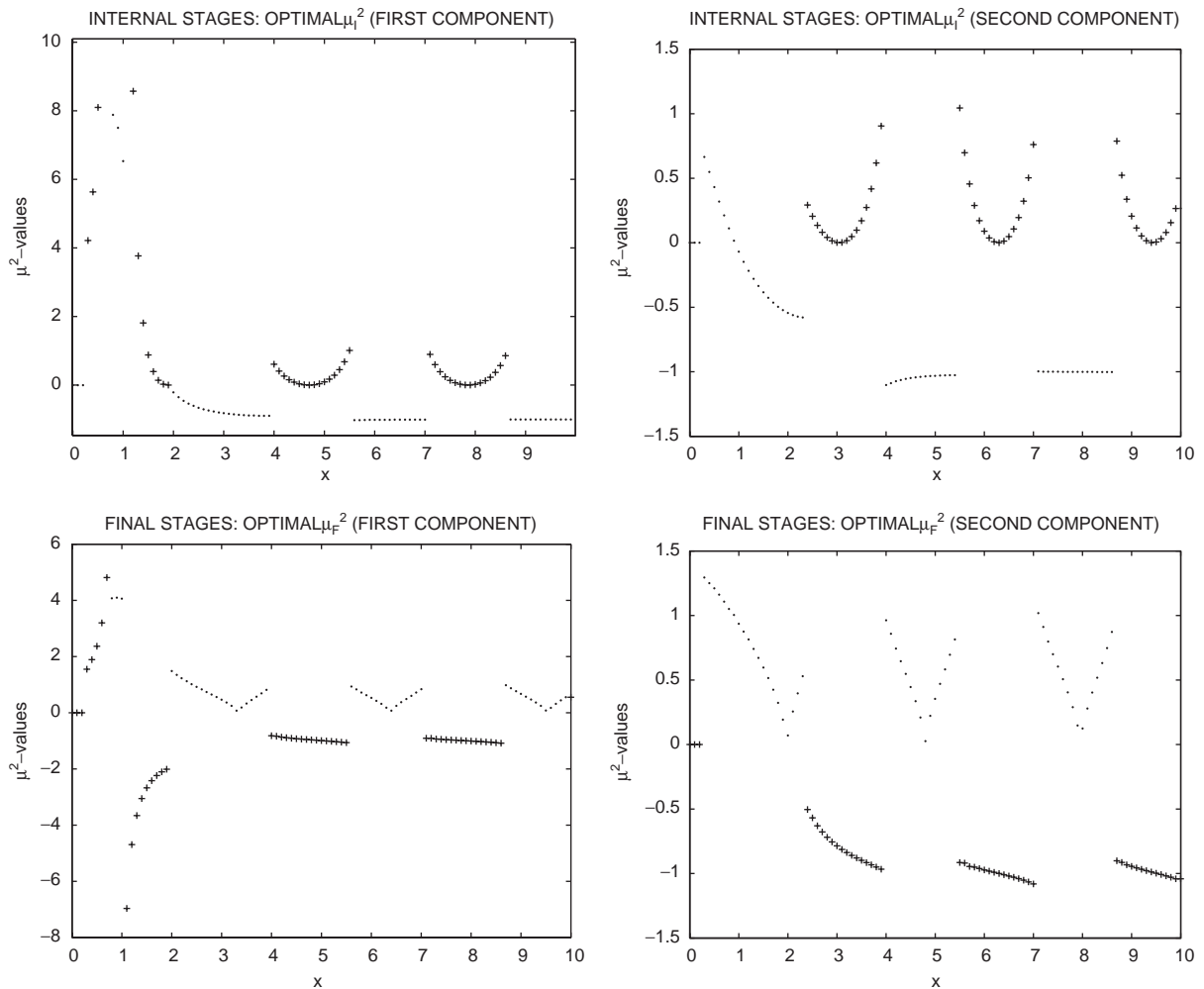


Fig. 3. Variation with x of the optimal μ^2 -values for both components of (6.3), for the internal stages (first row) and final stage (second row) in some integration points. Algorithm (ISA1, FSA2): crosses. Algorithm (ISA2, FSA1): points.

Problem 2. We consider the following nonlinear second-order ODE of Prothero and Robinson type:

$$y'' + v^2(y - g)^3 = g'', \quad g(x) = \cos(x), \quad y(0) = g(0), \quad y'(0) = g'(0). \quad (6.2)$$

This scalar problem can be written as a system of two first-order ODEs. The problem is solved in the interval $[0, 10]$ for $v = 10^4$.

Problem 3. We consider the system of two linear ODEs with eigenvalues -1 and β :

$$\begin{aligned} y_1' &= -2y_1 + y_2 + 2\sin(x), \\ y_2' &= -(\beta + 2)y_1 + (\beta + 1)(y_2 + \sin(x) - \cos(x)). \end{aligned} \quad (6.3)$$

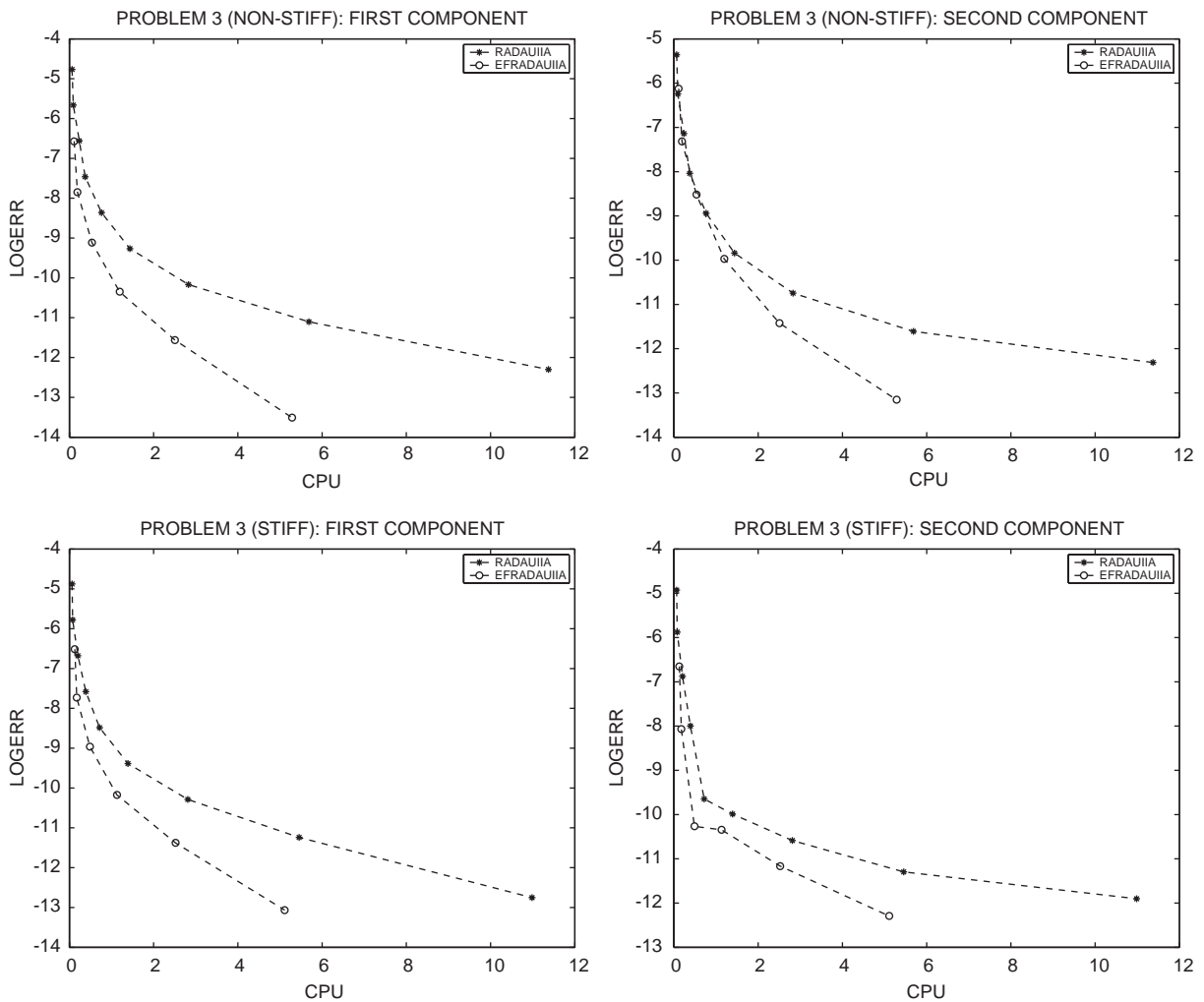


Fig. 4. Efficiency curves for the classical RadauIIA method and the optimal EFRadauIIA method applied to Problem 3 (6.3) in the cases $\beta = -3$ (nonstiff) and $\beta = -1000$ (stiff). The initial conditions are given by (6.5).

This system for $\beta = -1000$ first appears in [19] and it was used for the illustration of the phenomenon of stiffness. The system is also used in the papers [16,29] on frequency evaluation algorithms for EF methods. The analytical solution is given by

$$\begin{aligned} y_1(x) &= \chi_1 \exp(-x) + \chi_2 \exp(\beta x) + \sin(x), \\ y_2(x) &= \chi_1 \exp(-x) + \chi_2(\beta + 2) \exp(\beta x) + \cos(x), \end{aligned} \quad (6.4)$$

where χ_1 and χ_2 are arbitrary constants. The domain of numerical integration is $[0, 10]$. For the initial conditions

$$y_1(0) = 2 \quad \text{and} \quad y_2(0) = 3, \quad (6.5)$$

we obtain the values for the constants $\chi_1 = 2$ and $\chi_2 = 0$. It is remarkable that the solution becomes β -independent.

6.2. Illustrating the increase of the order of accuracy

In this subsection, the increase of the order of the method (from three to four) will be verified by Problem 3 with initial conditions (6.5). Just as in [16,29], we use the steplengths $h = 0.1, 0.05$ and 0.025 for $\beta = -3$ (a nonstiff case) and $\beta = -1000$ (a stiff case). Four optimal frequencies are involved since every component needs two different frequencies. The absolute errors at the endpoint from the classical RadauIIA and EFRadauIIA methods are presented in Table 1. It is clear that the optimal EFRadauIIA method is much more accurate than its classical companion. In Fig. 2 we draw the scaled errors $(y(jh) - y_j)/h^4$, $j = 1, 2, 3, \dots$ in each integration point in order to confirm that the new optimal EFRK method has order four. The variation of the optimal μ_L^2 and μ_F^2 at each integration point for both components are drawn in Fig. 3. The optimal frequencies for the internal stages are just the same as for the EF methods from [17,26]. This is a direct consequence from the fact that the stage-order of the two-stage RadauIIA method is equal to two which is also the order of the classical underlying methods from [17,26].

6.3. Illustrating the efficiency

To test the efficiency of the optimal EFRadauIIA method by Problems 1–3 we have compared the behaviour in fixed stepsize mode with the underlying classical RadauIIA method. For each problem we choose the steplengths $h = \frac{1}{10}, \frac{1}{20}, \dots, \frac{1}{10 \cdot 2^8}$ (classical RK method) and $h = \frac{1}{10}, \frac{1}{20}, \dots, \frac{1}{10 \cdot 2^5}$ (optimal EFRK method). We present the efficiency curves: accuracy versus the computational cost measured by the CPU time required by each code. For Problem 3 (nonstiff and stiff case) with initial conditions (6.5) the efficiency curves are drawn in Fig. 4. Now, we choose for Problem 3 (stiff case) other initial conditions such that the stiff part of the solution is present:

$$y(0) = 0 \quad \text{and} \quad z(0) = 1. \quad (6.6)$$

The efficiency curves for this problem and Problems 1 and 2 are displayed on Fig. 5.

For all the test problems we observe that the classical RK method and the optimal EFRK method have a comparable efficiency for steplength $h = \frac{1}{10}$. It is obvious that for smaller steplengths the optimal EFRK method is more efficient than the classical RK method. In this case we have showed that the extra computation time needed for the optimal EFRK method (estimation of the solution using the Milne–Simpson formula, determination of the higher order derivatives, calculation of the coefficients, ...) is negligible. Similar results are found for the optimal EFRK method from [29].

7. Conclusions

The main theoretical output consists in bringing new sensible arguments in favour of the idea that the applicability of EF methods is much larger than only for ODEs with oscillatory or periodic solutions [15–17]. We have developed a new optimal EFRK method for the numerical solution of stiff systems of first order ODEs. If step control is added to the above algorithms these methods can effectively be applied to real physical or physical–chemistry problems as described in the CWI test set [20]. Further investigations have

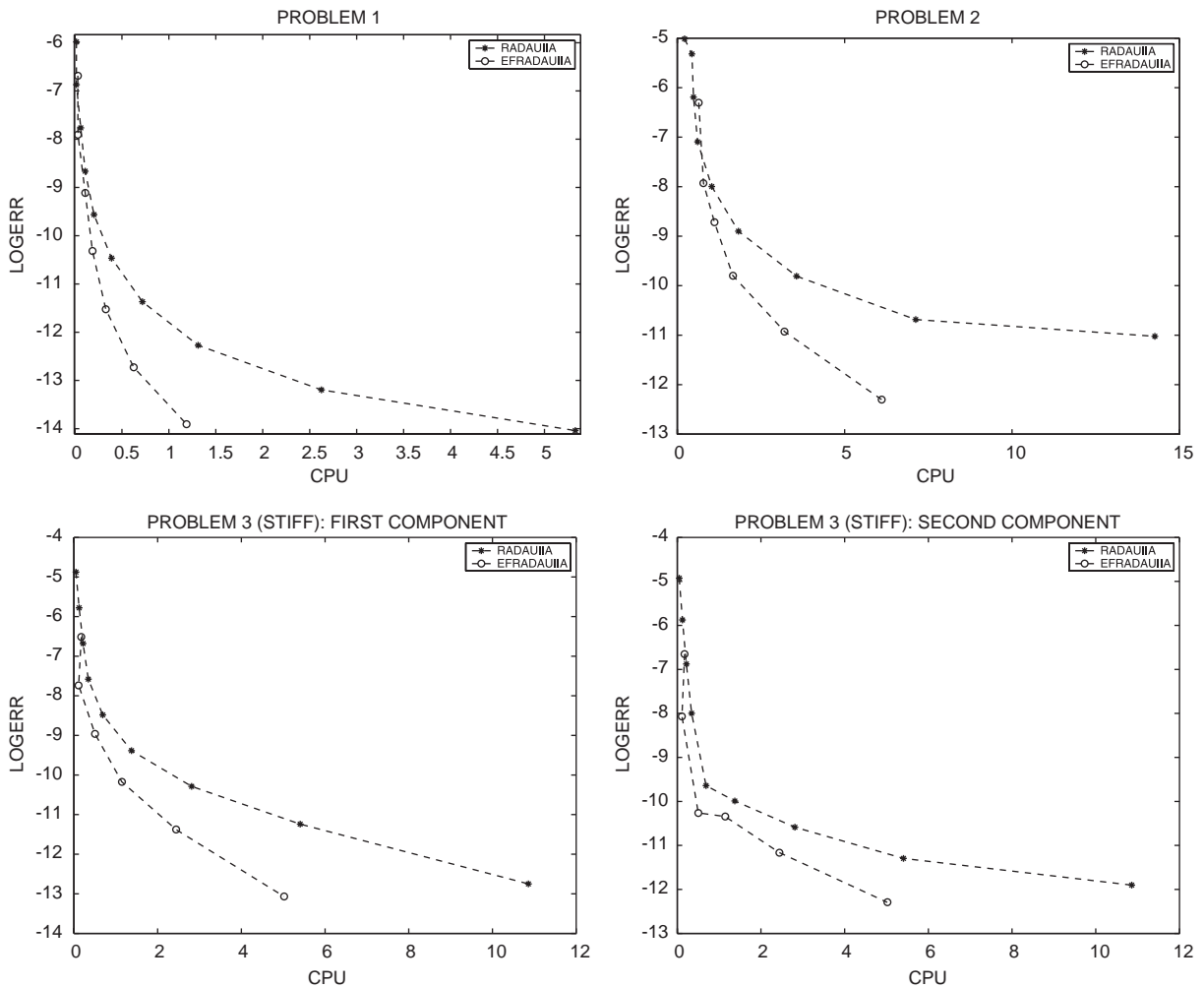


Fig. 5. Efficiency curves for the classical RadauIIA method and the optimal EFRadauIIA method applied to Problem 1 (6.1), Problem 2 (6.2) and Problem 3 (6.3) (stiff case). For the initial conditions of the latter problem we take (6.6).

been performed along the lines of the recently proposed frequency evaluation algorithm for EF multistep methods in [15–17]. In this paper, we have illustrated that a direct application of Ixaru's frequency evaluation algorithm is not possible for EFRK methods of order $p > 2$. In order to overcome some specific difficulties we have developed an efficient extension of Ixaru's frequency evaluation algorithm for some EFRK methods based on two different optimal frequencies.

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